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Tailoring the electronic properties of semiconducting nanocrystal-solids: InAs embedded in SnS_x matrices[1] EMILIO SCALISE, STEFAN WIPPERMANN, Max Planck Inst fuer Eisenforschung GmbH, GIULIA GALLI, DMITRI V. TALAPIN, The University of Chicago — Recent advances in wet chemical techniques enable the facile synthesis of nanocrystals (NCs) and their assembly into complex solid structures (NC-solids), offering exciting prospects for solar energy conversion, light emission and electronic applications. The properties of these composites are strongly determined by structural details at the NC/matrix interface and the composition of the embedding matrix. We carried out a systematic study of the interaction between InAs NCs and SnS_x matrices using a grand canonical *ab initio* thermodynamics approach to identify general trends for the stability of structural motifs possibly occurring at the NC/matrix interface. The resulting models have been used as a basis for *ab initio* molecular dynamics calculations to investigate the impact of different mass densities and stoichiometries on the internal matrix structure and the NC-solids' electronic properties. We demonstrate that both the NC-matrix interface and the internal regions of the matrix show complex structural features, depending on specific synthesis conditions. Thus to obtain a detailed understanding of experimental data it is necessary to take into account such complex interfacial and matrix-internal structures beyond simplified NC-solid models.

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